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On numerical flux evaluation using coupled reconstruction based on entropic redundant variables

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SUMMARY

This paper describes a novel approach to the simulation of conservation systems based on redundant variables constraints. This allows the imposition of more physical conditions to obtain a better determination of the reconstruction problem. The results achieved for a passive scalar transport and a Burgers equation test case are illustrated. Reported numerical simulations of simple 2D incompressible flows also indicate the good quality of the proposed approach. Copyright © 2005 John Wiley & Sons, Ltd.

KEY WORDS: entropic redundant variables; reconstruction

1. INTRODUCTION

The problem of constructing numerical schemes for the advective terms of balance equations endowed with good properties in terms of numerical dissipation is of great importance. This is particularly true in the case of large eddy simulations (see for instance Reference [1] where accurate analyses show that in some instances high-order schemes may fail to conserve kinetic energy) and Euler equations for which the consequences of the adopted reconstruction procedure on the associated balance of any entropic quantity have been often evidenced (see for instance Reference [2]). The aim of this work is to introduce a novel approach for the reconstruction procedure required for the calculation of numerical fluxes in control-volume (CV) techniques.

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2. PROJECTIVE METHODS

The time-dependent balance equations

$$\frac{\partial w^r}{\partial t} + \mathrm{div}(\underline{F}^r) = 0 \tag{1}$$

that, together with appropriate boundary conditions, model the transport phenomena are in general strongly coupled. However, often the space reconstructions of the balanced species $\langle w^r \rangle$ adopted at each discretized time t^n are uncoupled; indeed, these are usually based on data sets (e.g. the set of surrounding CV average values) exclusively and directly related to the variable to be reconstructed. The optimal choice of this set has been the object of several efforts (limiters theory, ENO and WENO schemes, etc.), aiming at ensuring such important qualities of the numerical schemes as the various *monotony* properties and/or the control of the total variation of the solution. Generally, the data adopted for the determination of the reconstruction parameters are assumed to be a set of linear functionals, e.g. projections, of the functions describing the quantity to be reconstructed. In the last case, the equations of the system (or part of it) that contribute to the determination of the reconstruction parameters are

$$\langle P_i^r(\underline{x}, \underline{a}_i^r), s_i(\underline{x}) \rangle = \langle w, s_i(\underline{x}) \rangle_i^r \triangleq \langle w \rangle_i^r \tag{2}$$

where r is the species index, i the space index of the local reconstruction, $\underline{x}$ is the space coordinate, P_i^r the reconstruction shape, $\underline{a}_i^r$ the reconstruction parameters and s_i the test function (e.g. a set function in CV_i). In general, it results that

$$\frac{\partial P_i^r(\underline{x})}{\partial \langle w \rangle_j^k} = \Phi(r, i, k, j)\, \delta_{rk} \tag{3}$$

so that the parameters $\underline{a}_i^r$ are determined independently for each r.

It is well known that, given a set of balance equations, a strong solution verifies an *induced* balance of some entropic species (ε^s) if a flux function for such entropic species can be defined (see for instance Reference [3])

$$\frac{\partial \varepsilon^s(w^r)}{\partial t} + \mathrm{div}(\underline{G}^s(w^r)) = 0 \tag{4}$$

while for weak solutions the entropic species does not verify the balance on the discontinuities, i.e. the Rankine–Hugoniot conditions.

Therefore it is possible, given the reconstruction of $\underline{w}$, to evaluate the numerical fluxes $G^s(w^r)$ of the entropic species $\varepsilon^s(w^r)$ as well as its time evolution. The role of such complementary computation is to furnish additional integral constraints for the new reconstructions of the balanced quantities. In fact, the integral constraints on the entropic variables may involve simultaneously the reconstructions of primitive variables as

$$\langle \varepsilon^s(\underline{w}(\underline{P}_i)), s_i(\underline{x}) \rangle = \langle \varepsilon \rangle_i^s \tag{5}$$

(where $\underline{w}(\underline{P}_i)$ indicate the required reconstructed vectors). Equations (2) and (5) constitute a coupled system of equations and the obtained reconstructions are also fully coupled.

The entropy-controlled (or—more in general—S norm-controlled) reconstructions are based on a technique for fixing K parameters (somehow connected to the shape P_i) by means of K' (with $K' \leqslant K$) constraints usually related to the average values $\langle w \rangle_j^r$ of the cells in the neighbourhood of the ith cell and to suitable estimates of the entropic values $\langle \varepsilon \rangle_i^s$.

If necessary (i.e. when one chooses to have $K' < K$), the K parameters are fixed by looking for optimal solutions in some sense (for instance, those corresponding to the Moore–Penrose generalized inverse). Therefore, such optimal solutions will have, in some norm, the minimal *distance* from any predicted reconstruction (that is a reconstruction guessed by means of any suitable information such as an estimate of the entropic variables deriving from their balance equations).

A discrete sub-cell implementation of the above-described procedure is advisable. Indeed, for the choice of the K parameters related to the reconstruction shape P_i better than a direct use of the K coefficients of a polynomial, it appears convenient to choose a piecewise constant approximation of the shape P_i itself. That is, a K-dimensional numerical vector $[u_1, u_2, \dots, u_k]$ will parametrically represent the reconstruction shape P_i. Thus, in general, if somehow predicted values of these parameters (i.e. K parameters corresponding to any *useful guess*—namely one with an appropriate entropy—of the required reconstruction) are available, let us say $[u_1^s, u_2^s, \dots, u_k^s]$, a suitably chosen optimal correction of the prediction $[\underline{u}^s]$, say $[\delta u_1, \delta u_2, \dots, \delta u_k]$, which satisfies the K' constraints, will produce a corrected vector:

$$[u_1, u_2, \dots, u_k] = [u_1^s, u_2^s, \dots, u_k^s] + [\delta u_1, \delta u_2, \dots, \delta u_k]$$

which will satisfy the classical K' constraints and will have the minimal *distance* from the vector approximating the *useful guess*.

3. NUMERICAL TESTS

In order to demonstrate the convenience of employing redundant or entropic non-independent quantity balances, some results obtained in simple 1D and 2D tests are reported, and some comments are appropriate here. First of all, we emphasize that—whichever approach is adopted—to improve time accuracy of the method, an estimate of the time integral of the convective flux of the transported quantity across the CV elementary boundary is taken into account by making use of a suitable space integral of the reconstructed function over the so-called *traversing region*, in the neighbourhood of each elementary boundary (more details on this point of view can be found, for instance, in Reference [4]). However, for these test cases, only a few of the very many possibilities described above have been adopted: the entropy function chosen for the *induced balance* is the square of the transported scalar, and for 1D cases, when *linear reconstructions* are chosen the two parameters are determined simply by imposing the constraints on the average values of both the main variable and its square (over a single, suitably chosen, CV), whereas when the scheme relies on *quadratic reconstructions*, the *guess* coefficients are obtained by a more or less classical reconstruction based on the average values of three suitably chosen cells (according to an upwind criterion) and the correction values are based on equations that compulsorily require that the cell average of the main balanced variable is recovered, while the recovering of the average values of the redundant entropic variable may be achieved in optimal ways. In 2D cases, piecewise quadratic reconstructions were performed involving five cell values according to Reference [5]. For

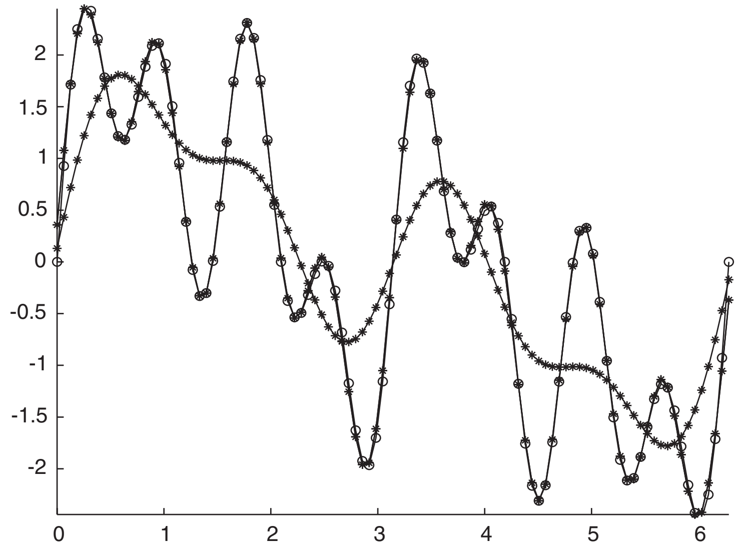

Figure 1. CFL = 0.3: +-+ entropy controlled; * * 3rd-order upwind; ∘∘ initial condition.

Navier–Stokes calculations, for the present, only a separate control on the components u^2 and v^2 has been implemented.

3.1. Passive scalar transport

The first test is the 1D passive scalar linear advection with periodic boundary conditions and is relative to an initial condition of a four harmonic components wave with wave numbers $k_0 = 2\pi/L$, $2k_0$, $4k_0$ and $8k_0$.

The numerical solution is relative to a third-order scheme for which the reconstructed functions are 2nd-degree polynomials obtained with the present approach and is compared with the one based on a *classical* third-order scheme. The results reported in Figure 1 are relative to a Courant number $c = 0.3$ and to a final travelling time corresponding to 100 wavelengths of the first harmonic, and clearly show the good properties of the proposed scheme in terms of numerical dissipation, i.e. the corresponding numerical solution is *practically coincident* with the analytical one, without any apparent dissipation or dispersion effect in contrast to the evident dissipation for the case of the *not* entropy-controlled third-order scheme.

3.2. The Burgers equation

The non-diffusive Burgers equation represents a classical and very interesting test case for numerical schemes of conservation problems.

Its non linear hyperbolic character is very useful to verify properties of shock capturing and monotony. One would like to be able to evaluate the *production term*—arising at the discontinuity—in the balance of the entropic variable (as indicated, for instance, in Reference [6]), but this, of course, is out of our scope. Moreover, in this case the already cited technique of the conversion of the time integrals of the cell boundary fluxes to space

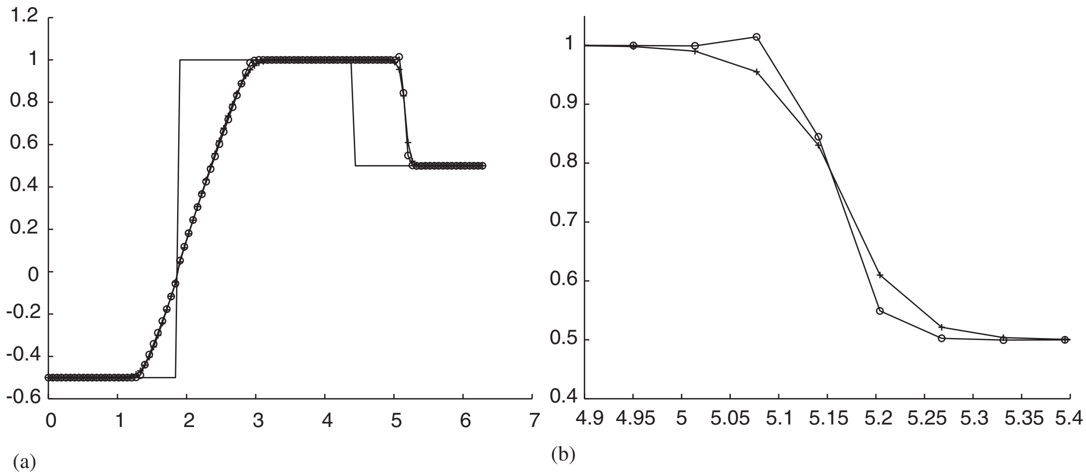

Figure 2. (a) Regular: Burgers equation: ∘∘ second-order entropy controlled; ++ second-order TVD; -- initial condition. (b) enlargement: Burgers equation: ++ second-order entropy controlled; ∘∘ second-order TVD.

integrals—due to the *non-linearity* of the fluxes—has been suitably modified. The test reported in Figure 2(a) illustrates the good quality of shock capturing for the present approach, although complete control of the energy dissipation mechanism at the discontinuity has not yet been reached; this obviously requires further development following the previously described procedure. In Figure 2(b), an enlargement of the shock region is reported for a more detailed comparison.

3.3. 2D channel flow

The developing flow at the entrance of a channel has been simulated in order to put in evidence the properties of the proposed approach in a Navier–Stokes computation. A flat inlet velocity profile has been assigned, while the outflow region is subject to regularized conditions. As is well known in this entrance region, there is an excess pressure drop with respect to the constant pressure gradient of the Poiseuille solution developed at the end of the duct. In Figure 3, the quantity $A=(P_x^{3\text{rd}}-P_x^{\text{Ent.cont.}})/P_x^{\text{mean}}$, namely the ratio of the difference between the streamwise pressure gradients computed with and without the present approach schemes to the local mean pressure gradient, is plotted in the entrance region at Reynolds numbers of 40, 80 and 100. The computations were performed on a Cartesian uniform grid. The positive values of A suggest that the entropy-controlled scheme achieves some reduction of the numerical dissipation.

3.4. 2D flow past a cylinder

Finally, calculations of the flow past a cylinder have been performed on rather coarse uniform grids, following the immersed boundary approach (a description of which can be found for instance in Reference [7]) and implementing a 2D version of the schemes with energy controlled reconstructions. The results of calculations are reported in Table I for Reynolds

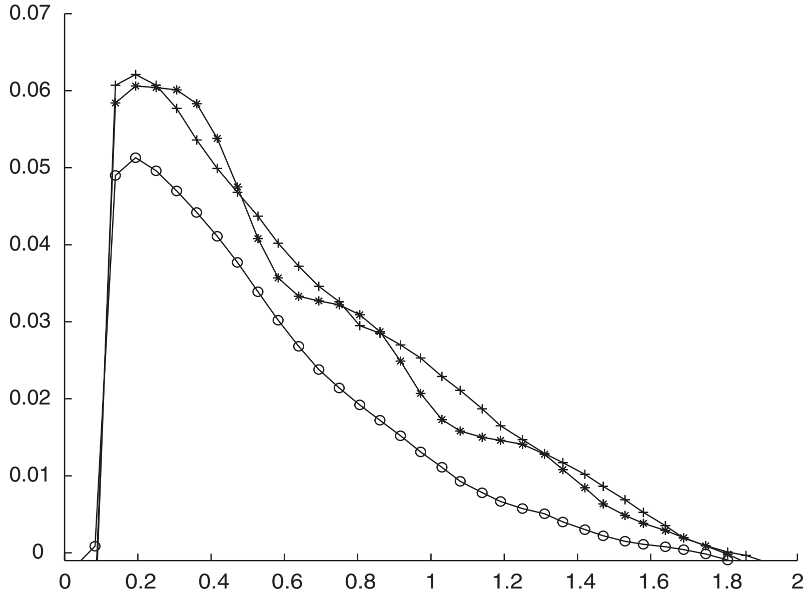

Figure 3. A; ○ ○ $Re = 40$; * * $Re = 80$; + + $Re = 100$.

Table I. Drag coefficient.

Re	C_d(entropy contr.)	C_d(3rd order)
100	1.63	1.60
200	1.35	1.29
500	0.98	0.87

number $Re = 100$, 200 and 500. A comparison of the drag coefficient C_d relative to companion computations accomplished by using—for the convective terms—third-order schemes with and without the energy-controlled reconstructions suggests, analogously to the previous test case, how the proposed technique allows less dissipative computations.

4. CONCLUSIONS

The use of *induced* redundant balances of *entropic* variables for the optimization of the reconstructions of transported variables in the frame of a CV technique has been proposed and implemented in a preliminary version. The good qualities of the proposed approach in terms of numerical dissipation have been illustrated through simple 1D and 2D computations. Techniques for a better localized control of the energy dissipation, which may result functional to a suitable treatment of the Euler equations, appear necessary and these require further developments to be pursued following the above indicated paths.

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